# "DEVELOPMENT OF NEW SYNTHETIC METHODOLOGIES FOR THE SYNTHESIS OF OXA & AZA –HETEROCYCLES AS AN ACTIVE MEDICINAL SCAFFOLD"

**SHORT RESUME OF THE PLAN PROPOSED**

**FOR INVESTIGATION FOR Ph.D. DEGREE**

**UNDER THE FACULTY OF SCIENCE**

*To be submitted To*

**Swami Ramanand Teerth Marathwada University, Nanded**

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**Format for submission of Ph.D. Synopsis / Work plan**

**For faculty of Science to be submitted in front of RRC**

# DEVELOPMENT OF NEW SYNTHETIC METHODOLOGIES FOR THE SYNTHESIS OF OXA & AZA –HETEROCYCLES AS AN ACTIVE MEDICINAL SCAFFOLD


## Abstract:

The Ph.D. research project focuses on the exploration of green chemistry principles in the synthesis of heterocyclic compounds, with a specific emphasis on their potential as active medicinal scaffolds. Heterocyclic compounds are widely prevalent in pharmaceuticals due to their diverse biological activities, and this research seeks to develop sustainable synthetic methodologies while evaluating the pharmacological significance of the synthesized compounds.


## Introduction:

The synthesis of heterocyclic compounds plays a pivotal role in pharmaceuticals, agrochemicals, and materials science [1]. However, traditional synthetic methods often come with environmental and sustainability challenges, necessitating a paradigm shift towards more eco-friendly approaches. Heterocyclic compounds are widely distributed in nature and many of these possess medicinal/biological/pharmacological activity. In addition to nature-derived heterocycles, a large number of synthetic heterocycles are being used as medicines [2]. In this context, the incorporation of green chemistry principles emerges as a promising solution [3]. This introduction aims to explore the significance of adopting a green chemistry approach in the synthesis of heterocyclic compounds, shedding light on its potential to mitigate environmental impact while maintaining the efficiency and versatility required in modern chemical processes.

The imperative for a sustainable and environmentally conscious approach to heterocyclic compound synthesis stems from the recognition of the adverse effects associated with conventional methods. Traditional techniques frequently involve the use of hazardous solvents, high energy consumption, and the generation of copious amounts of waste. As society increasingly prioritizes environmental responsibility, the need for alternatives becomes more pronounced.

This introduction delves into the rationale behind embracing a green chemistry approach in heterocyclic compound synthesis, underscoring its potential to revolutionize the field by aligning chemical practices with sustainable principles. Use of safer solvents satisfies green chemistry practices. [4] From the green chemistry perspective, the best solvent for reactions is no solvent. However, this ideal situation is not always achievable and choice of more eco-friendly solvents becomes critical [5-7]. Through the exploration of green methodologies,

this synopsis aims to illuminate a pathway towards more responsible and eco-friendly synthetic strategies, fostering a harmonious coexistence between scientific advancements and environmental stewardship**.**

## Review of Literature:

Through the exploitation of several conventional strategies in sub disciplines of chemistry and the molecular sciences became challenging due to toxic chemicals in last few years. As a result, there is a growing appreciation towards the newly emerging field of green chemistry which is required as an avenue for sustainable development of heterocyclic derivatives over conventional techniques with improved therapeutic efficacy. [8]

Several green chemistry-based synthetic methods like multi-component single pot reaction, recyclable green-based catalyst, green solvent, reusable solvent, ultrasound-mediated synthesis, the solvent-free and microwave-assisted technique have been developed. [9]. Synthesis of heterocyclic compounds containing N, O and S heteroatom in their cyclic structures and has exhibited wide varieties of their biological activities. [10]

Various heterocyclic compounds like oxazole [11], thiazole [12], benzimidazole [13], Thiadiazole [14], fluroquinolone derivatives [15], Piperazine [16], Pyrimidone based heterocyclic compounds [17] possess pharmaceutical values.

## Objectives:

1. To design and execute a green synthesis route for heterocyclic compounds, emphasizing the use of renewable resources and environmentally friendly reagents.

2. To evaluate the efficiency and purity of the synthesized heterocyclic compounds through analytical techniques such as NMR spectroscopy, mass spectrometry, and chromatography.

3. To assess the environmental impact and sustainability of the developed synthetic route.

4. Study the biological activities such as antibacterial, antifungal, anti-cancer of synthesized heterocyclic products.

5. To develop and study the various techniques, methods for preparation of heterocyclic compounds.

6. Provide valuable information on the pharmacological activities and potential medicinal applications of the synthesized heterocyclic scaffolds, contributing to drug discovery efforts.

7. Establish correlations between the chemical structures of synthesized compounds and their biological activities, aiding in the rational design of future drug candidates.

8. Try to replace traditional solvents with green solvents, PEG, Ionic liquids to increase the efficacy of reactions.

9. Publication of research papers in reputed national and international journals.

## Methodology:

The research will involve the selection of starting materials with a focus on readily available and sustainable feedstock's. Green synthesis techniques, including microwave-assisted synthesis, solvent-free reactions, and the use of catalysis, will be explored to minimize energy consumption and waste generation. The choice of solvents and reagents will be guided by their environmental impact, aiming for bio-based and non-toxic alternatives.

## Characterization:

The synthesized heterocyclic compounds will be characterized using advanced analytical techniques such as IR, NMR spectroscopy and mass spectrometry to confirm their structures and assess purity. Chromatographic methods will be employed to separate and purify the reaction products.

## Significance and Potential Applications:

The successful implementation of this green synthesis approach for heterocyclic compounds has the potential to contribute significantly to sustainable and environmentally responsible chemical synthesis. The synthesized compounds may find applications in pharmaceuticals, agrochemicals, and materials science, aligning with the growing global emphasis on green and sustainable technologies.

## Year-wise Plan of work / proposed work plan

**First Year**

- Literature survey and completion of course work.
- Study of various organic reactions related to heterocyclic compound synthesis with green chemistry approach.
- Designing of methods or techniques for the synthesis of heterocyclic compounds.
- Experimental study of various catalysts for the synthesis heterocyclic compounds with green chemistry approach.

**Second year**

- Study and development of various organic reactions.
- Synthesis of oxazole derivatives, Thiadiazole derivatives, piperazine derivatives, quinazoline, rifampicin derivatives, coumarin derivatives, thiazolidinone derivatives etc.
- Characterization and conformation of structure of products using IR, NMR, Mass spectroscopy
- Attend and presentation of research papers in National and International conferences.

**Third Year**

- Antibacterial study of newly synthesized heterocyclic compounds against various bacterial and fungal pathogens.
- Preparation and submission of results obtained in the journals of National/ International repute.
- Publication of research papers in the journals.
- Writing and Submission of thesis.

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